A NEW APPROACH TO TEMPERATURE SHIFT FUNCTIONS IN MODELING COMPLEX MODULUS DAMPING DATA

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ABSTRACT

A new approach to determining the temperature shift function and its utility in smoothing, interpolating, and modeling a set of complex modulus data are described in detail and examples are given. A set of experimental data to characterize the dynamic mechanical properties of a viscoelastic damping polymer typically includes the real component of complex modulus and the material loss factor as well as the experimental frequency and temperature. The set of data must be made useful for design purposes. The present approach analytically represents the wicket plot loss factor as a function of the modulus magnitude. A ratio of polynomials is then used to model the complex modulus as a function of reduced radian frequency. The perpendicular distance from each experimental point to the wicket plot is used to calculate the temperature shift function.

KEY WORDS: viscoelastic, vibration, noise, control, damping, complex modulus

INTRODUCTION

There have been a growing number of successful, high-payoff service applications of viscoelastic damping materials for vibration and noise control. A crucial factor in the further advancement and application of damping technology is accurate and efficient smoothing, interpolation, modeling (SIM), presentation, retrieval and dissemination of damping material design data[1,2,3]. The present document purports to improve the SIM state of the art. Most sets of data for dynamic mechanical properties of damping materials are generated for screening purposes or for engineering applications and therefore, typically and justifiably, do not cover temperature and frequency ranges in a scientific manner. It is challenging to interpret the data in such a way as to be useful to the designer while providing a reliable indication of limitations.

Viscoelastic material of present interest undergoing stress and strain is treated as a linear system. Consequently, a well-established body of mathematics from servomechanism feedback control systems applies. Specifically, the real and imaginary components (or any other pair) of complex modulus (actually a frequency response function) must satisfy a certain mathematical interrelationship. A new model (the “Ratio Model” or just “Ratio”) of the complex modulus as a function of reduced frequency is used, namely, ratios of factored polynomials of integer order, and the individual factors are of first order, while the numerator and the denominator are of the same order. One pair of first order factors, one in the numerator and the other in the denominator, result in one "step" with respect to Bode Diagram considerations. The Ratio Model intrinsically guarantees that the above interrelationship is satisfied.

Historically, the wicket plot has been introduced in order to edit individual points and check for an obvious lack of quality/accuracy. With respect to the present approach, the wicket plot actually displays two components of the CM, namely the material loss factor and the magnitude (or real part) of the modulus. The present approach is based on evaluating parameters in the Ratio Model such that the interrelationship established by the wicket plot are maintained. The form of the Ratio Model has been selected for ease of fitting the wicket plot by initialization and iteration and for ease of interconversion between any one dynamic mechanical property and any other.

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE **2004**	2. REPORT TYPE	3. DATES COVERED **00-00-2004 to 00-00-2004**
4. TITLE AND SUBTITLE **A New Approach to Temperature Shift Functions in Modeling Complex Modulus Damping Data**		5a. CONTRACT NUMBER 5b. GRANT NUMBER 5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)		5d. PROJECT NUMBER 5e. TASK NUMBER 5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **CSA Engineering,2565 Leghorn Street,Mountain View,CA,94043**		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S) 11. SPONSOR/MONITOR'S REPORT NUMBER(S)
12. DISTRIBUTION/AVAILABILITY STATEMENT **Approved for public release; distribution unlimited**		
13. SUPPLEMENTARY NOTES **The original document contains color images.**		
14. ABSTRACT **see report**		
15. SUBJECT TERMS		

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**		**16**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

Once the values of the parameters of the Ratio Model are established, the set of complex modulus data has been modeled as a function of reduced radian frequency with no knowledge of the temperature shift function (TSF) being required. Implicitly, each point on the arc length of the wicket plot is associated with a value of reduced radian frequency. To evaluate the temperature shift function for each experimental data point, the perpendicular distance from the point to the wicket plot determines an associated value of the reduced radian frequency. Knowing the associated value of the reduced radian frequency and the experimental frequency and temperature enables the calculation of the TSF for that point.

The present approach is interactive and highly automated and exploits modern computational power. This contrasts with the historical approach of defining the TSF visually (or perhaps with analytic geometry), for which least three decades of experimental frequency coverage for each experimental temperature is highly desirable, which requires considerable experience, and is extremely time consuming.

THE BASIC FRACTIONAL MODEL

Many viscoelastic damping materials have a rubbery plateau, a transition region (where the modulus changes rapidly and the loss factor reaches a maximum), and a glassy plateau. The basic fractional complex modulus equation[4,5], which possesses these characteristics, is

$$G(j\omega_R) = \left[G_e + G_g\left(j\omega_R/\omega_{RO}\right)^{\beta}\right] / \left[1 + \left(j\omega_R/\omega_{RO}\right)^{\beta}\right] \tag{1}$$

where the form of the parameters has been chosen to facilitate physical and mathematical interpretation. This expression is plotted in Figure 1. The expression for the exponent

$$\beta = \left(\frac{2}{\pi}\right)\arctan\left\{\eta_{\max}\left[\frac{\left(1-C^2\right)+2(1-C)C^{1/2}\left(1+\eta_{\max}{}^2\right)^{1/2}}{(1-C)^2-4C\eta_{\max}{}^2}\right]\right\}; C = G_e/G_g \tag{2}$$

is useful. The basic fractional calculus model for CM is extremely valuable for a crucial step in the present effort. A value for reference frequency which is reasonably close to that of many service applications

$$f_{REF} = 100Hz; \omega_{REF} = 200\pi \sim rad/\sec \tag{3}$$

is used in the present effort.

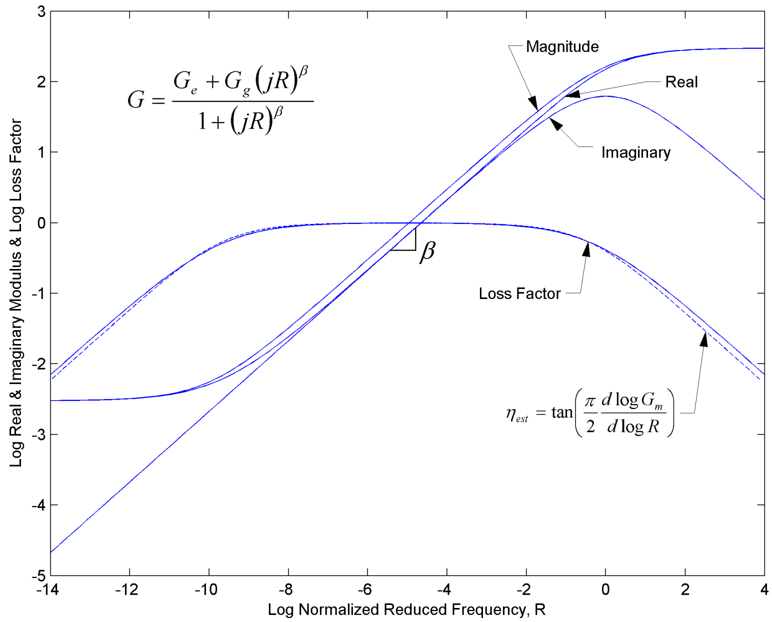

Figure 1: The Basic Complex Modulus Model

SOME PROPERTIES OF LINEAR SYSTEMS

Consider a single input, single output, causal, linear, constant-coefficient, stable, finite system and its associated frequency response function (FRF) in the form

$$H(f) = e^{-A} e^{j\delta}; \ln \mathrm{H} = -\mathrm{A} + j\delta \tag{4}$$

It is well known that if one component (i.e., magnitude, phase, real or imaginary) of the FRF is specified over the entire frequency range, any other may be obtained from the one given. This relationship is believed due originally to Kramers and Kronig[6, 7, 8]. The form of the CM model to be selected below will intrinsically guarantee that this property will be satisfied; this is a crucial point in the present work.

From the properties of systems, it is known that the loss factor is approximately proportional to the slope of both the modulus magnitude. With reference to Eqn 4, an equation useful for the present purpose is[9]

$$\begin{aligned}\delta(\omega_d) &= (\pi/2)|d\mathrm{A}/du|_0 + \\ &(1/\pi)\int_{-\infty}^{+\infty} \left[|d\mathrm{A}/du| - |d\mathrm{A}/du|_0\right] \ln \coth|u/2|\, du\end{aligned} \tag{5}$$

where

$$u = \ln(\omega/\omega_d) \tag{6}$$

An element of viscoelastic material may be considered to be a linear system with input of stress and output of strain or vise versa and the complex modulus is a FRF. By examining Eqn 4, it may be seen that

$$G_M = e^{-A}; \ln G_{\mathrm{M}} = -\mathrm{A}; dA/du = d\ln G_{\mathrm{M}}/d\ln\omega \tag{7}$$

and, because the integral term is small, (Note that ω and ω_R are interchangeable in most of these relationships)

$$\delta \approx (\pi/2) d \log G_{\mathrm{M}} / d \log \omega \tag{8}$$

from which[10],

$$\eta \approx \tan[(\pi/2) d \log G_{\mathrm{M}} / d \log \omega] \tag{9}$$

A numerical evaluation of this approximation is included in Figure 1.

THE MODEL FOR COMPLEX MODULUS

After extensive experience in fitting sets of complex modulus data, the model selected is a ratio of factored polynomials of integer order, where each factor is of the first order and the numerator and denominator are of equal order. One pair of first order factors, one in the numerator and the other in the denominator, result in one "step" with respect to Bode Diagram considerations. It happens that this form is particularly convenient for interconversion to other dynamic mechanical properties. Furthermore, Bode diagram considerations lead to convenient iteration algorithms in determining values for the parameters. Modern computational power is used to great advantage

$$G(j\omega_R) = G_e \prod_{i=1}^{\mathrm{N}} (1 + j\omega_R/z_i) \Big/ (1 + j\omega_R/p_i); z_i < p_i \tag{10}$$

See Figure 2. It is convenient to rewrite this equation in terms of r_i, which determines the location of the center of the riser, and a_i which determines the height of the riser

$$G(j\omega_R) = G_e \prod_{i=1}^{\mathrm{N}} (1 + j\omega_R a_i/r_i) \Big/ (1 + j\omega_R/a_i r_i) \tag{11}$$

the parameters are related by

$$p_i = a_i r_i; z_i = r_i / a_i; r_i^2 = p_i z_i; a_i^2 = p_i / z_i \tag{12}$$

This equation is called the “Ratio Model” and inherently satisfies the real-imaginary component relationship; this is vital to the present approach. Eqn 10 is a frequency response function and the associated transfer function is

$$G(s_R) = G_e \prod_{i=1}^{N} (1 + s_R / z_i) \Big/ (1 + s_R / p_i) \tag{13}$$

If Eqn 13 is divided by s_R, the method of partial fractions and the heaviside expansion formula (see any text covering laplace transforms) may be applied; the result is then multiplied by s_R to give a sum of fractions

$$G(s_R) = G_e + \sum_{i=1}^{N} (G_i s_R / p_i) \Big/ (1 + s_R / p_i) \tag{14}$$

where

$$G_k = -G_e \prod_{l=1}^{N} (1 - p_k / z_l) \Big/ \prod_{\substack{l=1 \\ l \neq k}}^{N} (1 - p_k / p_l) \tag{15}$$

which may be placed in the form

$$G_k = G_e\left(a_k^2 - 1\right)\prod_{\substack{l=1 \\ l\neq k}}^{N}\frac{1 - a_k a_l r_k /(r_l)}{1 - a_k r_k /(a_l r_l)} \tag{16}$$

The transfer function for the relaxation modulus is easily found from Eqn 14 [11]

$$G_{RLX}\left(s_R\right) = G\left(s_R\right)/\, s_R = G_e / s_R + \sum_{i=1}^{N} G_i /\left(p_i + s_R\right) \tag{17}$$

and, its inverse *LT* leads to the relaxation modulus

$$G_{RLX}\left(t_R\right) = G_e + \sum_{k=1}^{N} G_k e^{-p_k t_R} \tag{18}$$

Shapery had success in representing the relaxation modulus with this expression, which is a Prony series.

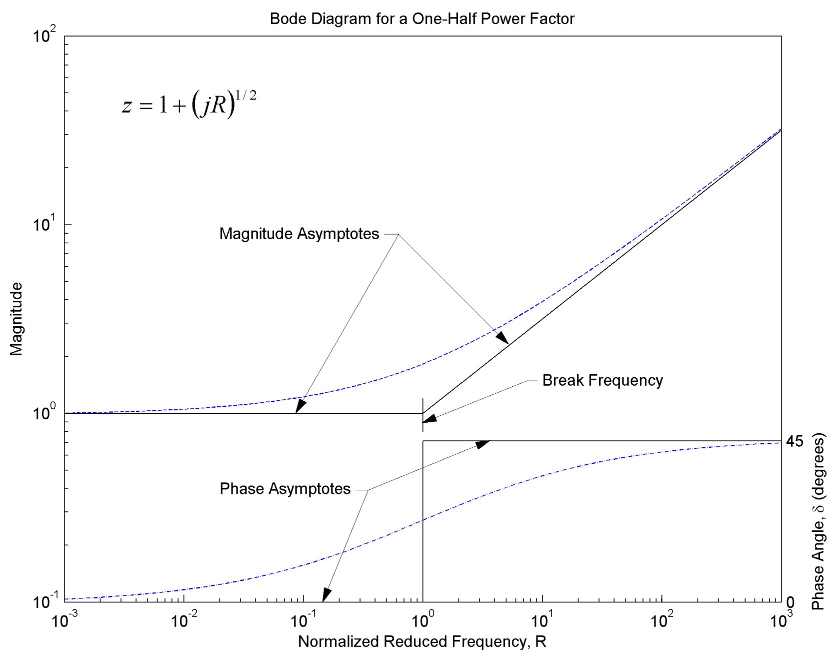

Figure 2: Conceptual Bode Diagram for the Ratio Model

THE WICKET PLOT

The first step in processing any set of complex modulus data is to examine the collection of experimental points in the wicket plot format, which is $\log \eta_G$ vs. $\log G_R$. Although $\log G_R$ is often displayed because it is of interest during design applications, $\log G_M$ is used for Bode plot visualization and in the calculations. If the set of data represents a thermorheologically simple (TRS) material, does not require a vertical shift of modulus for temperature and/or density, and has no scatter, the collection of data points will plot as a curve of vanishing width. Each location along the arc length, s, of the curve corresponds to a unique value of reduced radian frequency; however, this consideration is postponed until after the mapping step below. The material loss factor and the real modulus are cross-plotted in the wicket plot, and the reduced radian frequency, temperature, and frequency parameters do not appear. No part of any scatter in the wicket plot can be attributed to an imperfect temperature shift or modeling. The wicket plot may possibly reveal valuable information regarding scatter in the experimental data. The width of the band of data, as well as the departure of individual points from the band, are indicative of scatter. Acceptable scatter depends on the application. Nothing is revealed about the accuracy of measurements or about any systematic error. Low scatter in a wicket plot is a necessary but not a sufficient condition of data quality. Consistency does not indicate accuracy.

Ideally, the wicket plot would be maintained current as the set of data is being gathered in order to ensure adequate ranges of temperature and frequency as well as a possible real time indication of data quality problems.

After the set of data is accepted, an "Analytical Wicket" is developed as the next step to the smoothing, interpolating, and modeling (SIM) process. The range of experimental data on the wicket plot is represented by a series (approximately 15) of cubic splines. After the data region is characterized, the model Eqn 11 cannot be truncated because of considerations of Eqn 5. A "graceful/reasonable" extrapolation of the skirts of the wicket plot beyond the range of experimental data is essential. At present, a set of splines is used in the rubbery skirt region from the last data knot to a knot with loss factor two decades less and the slope gradually changing. A similar set is used in the glassy skirt region. The combined set of splines (i.e., rubbery skirt, data region, and glassy skirt) serve to define uniquely and precisely the loss factor as a function of modulus magnitude as well as to smooth and interpolate the data and is called the "Analytical Wicket." It is intended to be a good representation of the center and of the slope for the band of data and an appropriate extrapolation into the skirts. The maximum value of the Analytic Wicket defines the $\eta_{\max}$ and the associated $G_{M_{\eta_{\max}}}$. Furthermore, consistent with Eqn 3, the numerical value for the reduced radian frequency associated with this point will be assigned later is this process to be identical to that of the reference reduced radian frequency, 200π rad/sec (see Figures 3-5).

The Analytic Wicket is taken as the definition of the data in so far as the relationship between material loss factor and the modulus is concerned and serves as a constraint in the determination of values for the parameters in the Ratio Model. The individual experimental points will be used later in determining the TSF.

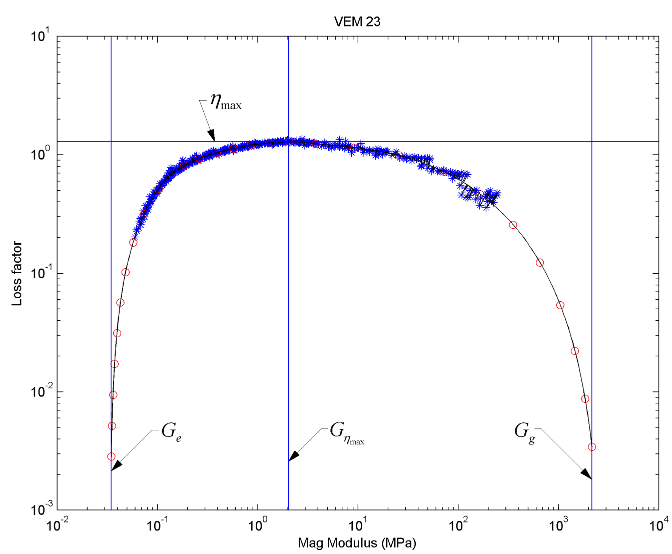

Figure 3: Analytic Wicket for VEM 23

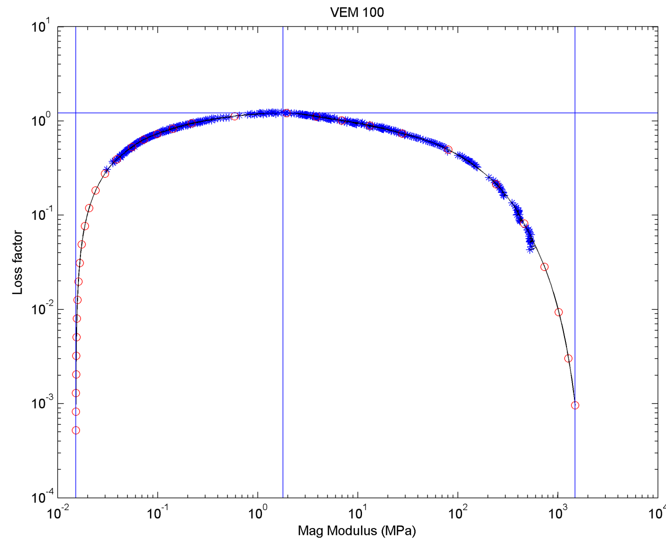

Figure 4: Analytic Wicket for VEM 100

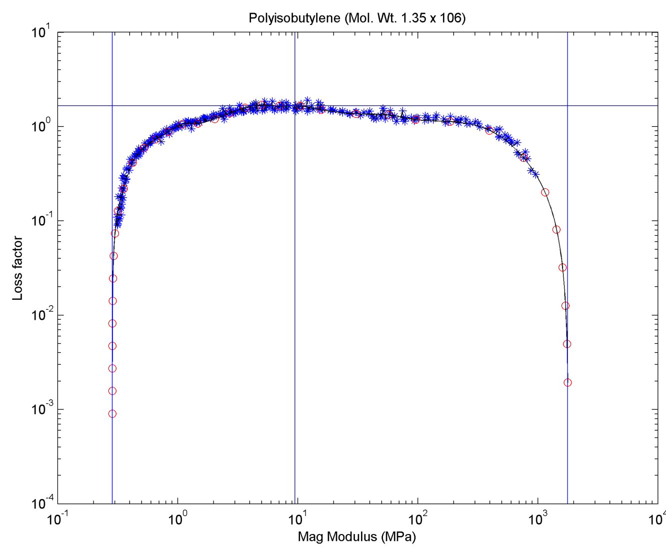

Figure 5: Analytic Wicket for Polyisobutylene

MAPPING

The x-y trajectory of a thrown ball is used as an example of mapping and is illustrated by Figure 6. Imagine that a set of tabulated x-y displacement data from a multiple stroboscopic photographic exposure through a window is available. The set of data may be cross plotted in the x-y domain without regard to time. Analytic geometry may be used to describe the trajectory in the x-y domain, and also if desired, to describe x and y as functions of the arc length of the trajectory. From physics, the equations of x and y as functions of time are known in terms of parameters whose values may be determined from experimental data. The arc length of the trajectory may be mapped into time and is justified by consideration of physics.

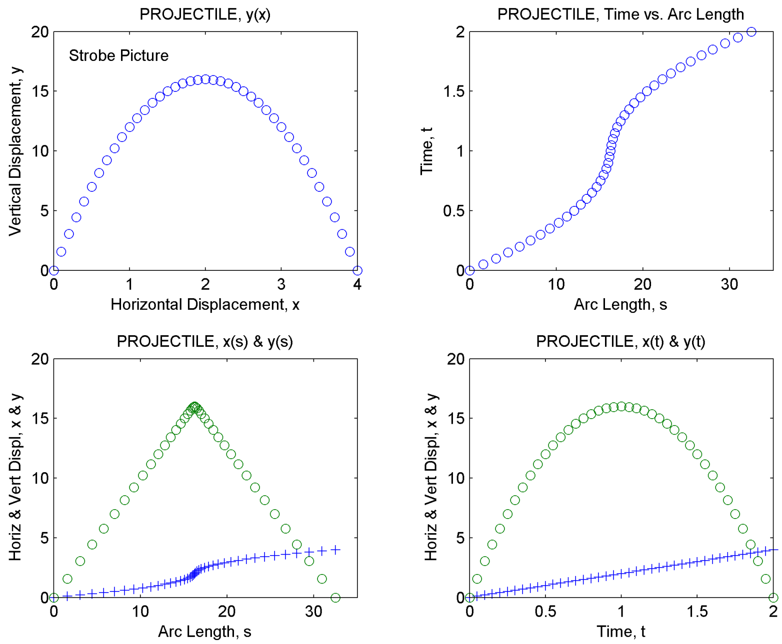

Figure 6: Projectile Parametric Illustration

Similar to the trajectory, the arc length of the wicket plot may be mapped into reduced radian frequency and is justified by the mathematical properties of systems. The basis of the mapping is the real-imaginary (or any other two components) relationship of linear systems. The form of the Ratio Model is particularly amenable to the mapping and rapid convergence.

The mapping consists of first initiation and then iteration until convergence. Eqn 11 using the r_i's and a_i's has been found to be most convenient; the r_i's are equally spaced on the log reduced radian frequency, ω_R, and do not change during the iteration.

The set of initial estimates of parameter values for the Ratio Model is determined by evaluating E1 at each Bode diagram step (i.e., at the center of each ratio of an associated pair of factors) in the model. The value for $\eta_{\max}$ is from the Analytic Wicket and the effective beta exponent is calculated. The Ratio Model with initial values of parameters is shown in Figure 7.

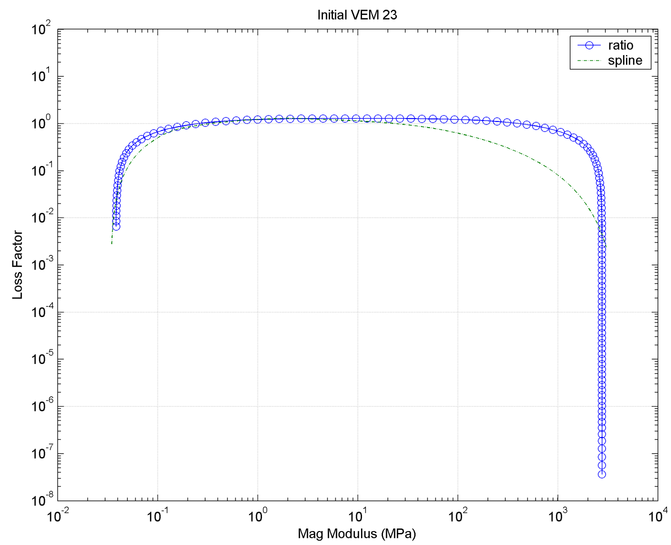

Figure 7: Ratio Initialization Wicket Plot for VEM 23

Iteration is based on Equation 5 approximated by Eqn 9; the loss factor is strongly dependent on the local slope of the magnitude. With reference to Figure 8, r_i indicates the location of the center of a vertical strip/slice with associated values for the magnitude and loss factor from the Ratio Model. The horizontal and vertical axes do not change and the curves are on a stretchable/compressible transparent layer portions of which also possibly slides right and left and/or up and down as a rigid body. If the slope of modulus within the strip is increased (by increasing the value for a_i), the Ratio loss factor would be increased.

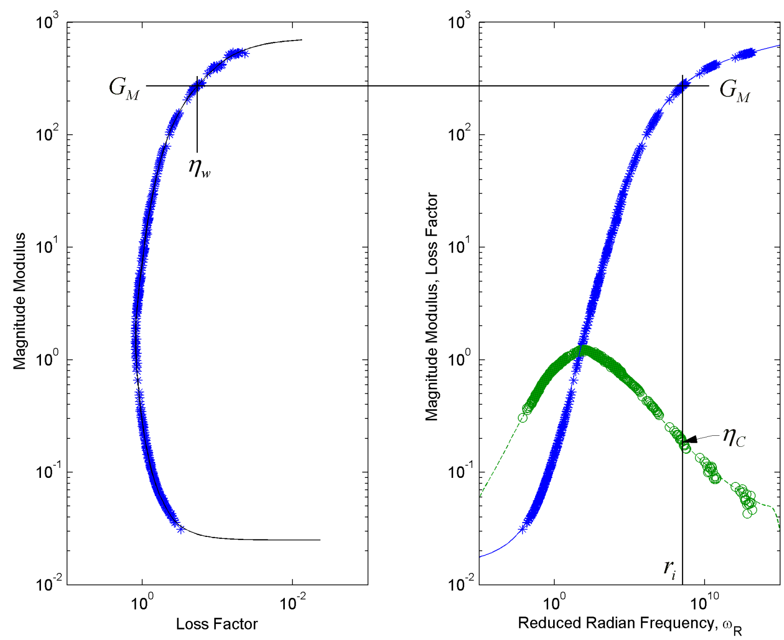

Figure 8: Illustration of Iteration Algorithm

In present practice, iteration consists of calculating the modulus magnitude and loss factor given by the Ratio Model at each value of r_i, calculating the loss factor from the Analytic Wicket associated with the value of the Ratio Model modulus, comparing the ratio model loss factor to the wicket loss factor, and adjusting the value of the a_i's to make the Ratio loss factor value more closely agree with that of the Analytic Wicket. The new a_i is approximated by Eqn 9 in terms of the old a_i, the loss from the Ratio, and the loss from the Wicket, but only a fraction, F, of the indicated change is made during each iteration pass. Bode diagram visualization provides guidance on this adjustment algorithm.

Convergence has been achieved when the values for the parameters in the Ratio Model do not change significantly with successive iterations; hopefully the Ratio Model matches the Analytic Wicket very closely (see Figure 9).

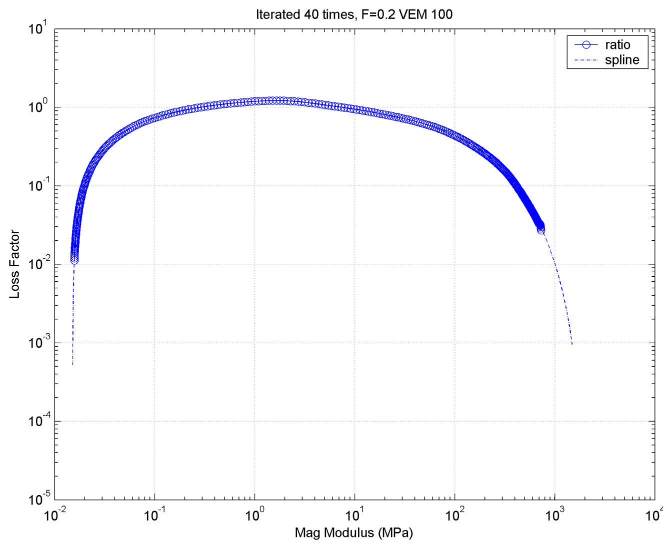

Figure 9: Ratio Converged Wicket Plot for VEM 100

After convergence, all of the r_i's are changed by a constant multiplier in order to cause $G_{M_{\eta_{\max}}}$ to occur at the reference reduced radian frequency, $\omega_{REF} = 200\pi$. This causes the temperature for which the value of the temperature shift function (yet TBD) is one to be the temperature for which the loss factor is the maximum for the reference 100 Hz cyclic frequency.

At this juncture, the smoothing, interpolating, and modeling of the complex valued modulus as a function of reduced radian frequency is complete and the frequency and temperature of the data points have not yet been considered. Furthermore, the arc length of the Analytic Wicket has been implicitly mapped into reduced radian frequency; i.e., a unique value of reduced radian frequency is associated with every value of arc length.

THE TEMPERATURE SHIFT FUNCTION DATA POINTS

The value of reduced radian frequency associated with each experimental data point may be found by considering the perpendicular distance to the wicket plot as illustrated in Figure 10. Given the experimental temperature, the experimental frequency, and the reduced radian frequency associated with each complex modulus data point, the temperature shift function (TSF) may be calculated.

$$\alpha_{\mathrm{T}}\left(\mathrm{T}_{\mathrm{E}_i}\right) = \omega_{R_i} / 2\pi f_{\mathrm{E}_i} \tag{19}$$

This is a totally new method of determining the temperature shift function (TSF). See TSF points in Figures 11-13.

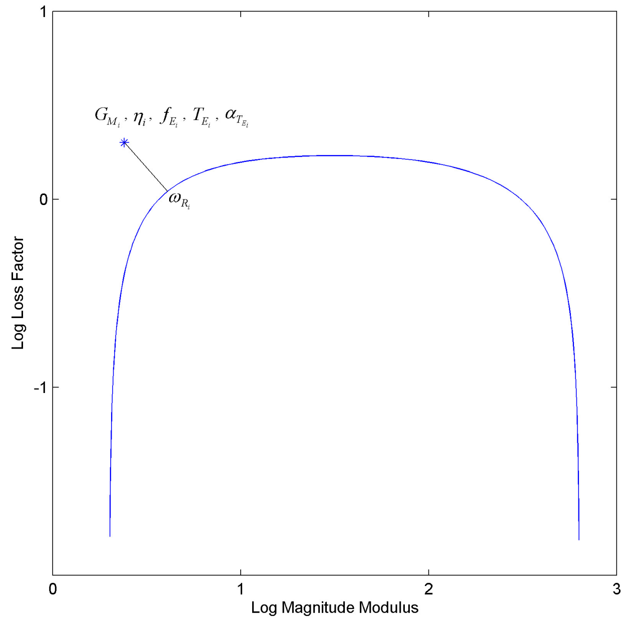

Figure 10: A New Method to Determine the Temperature Shift Function

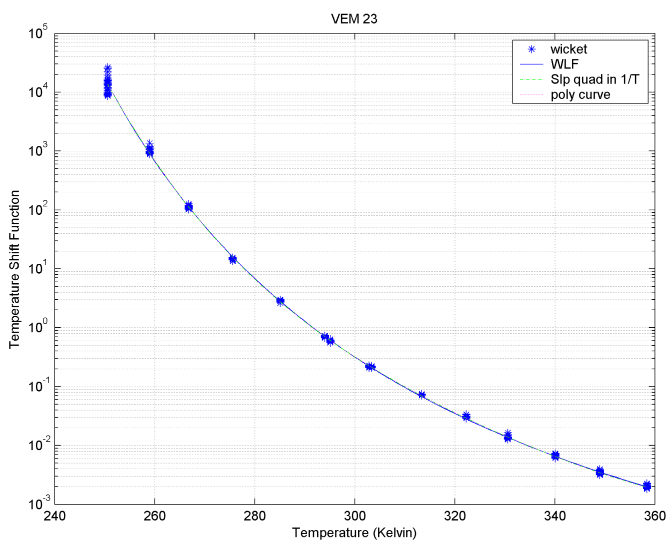

Figure 11: The Temperature Shift Function for VEM 23

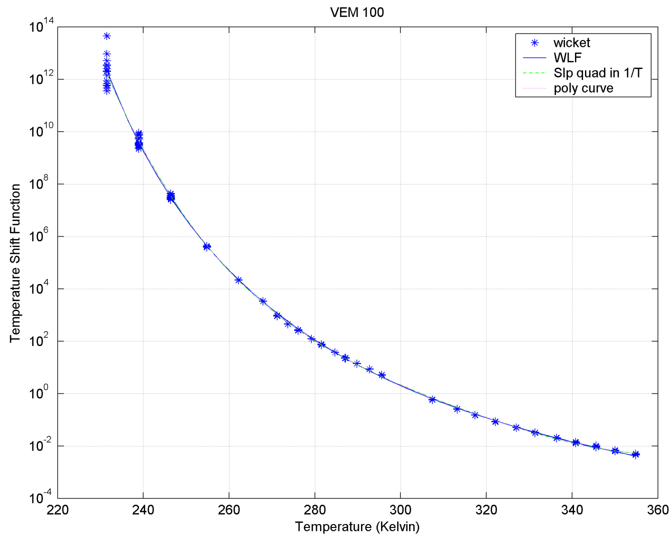

Figure 12: The Temperature Shift Function for VEM 100

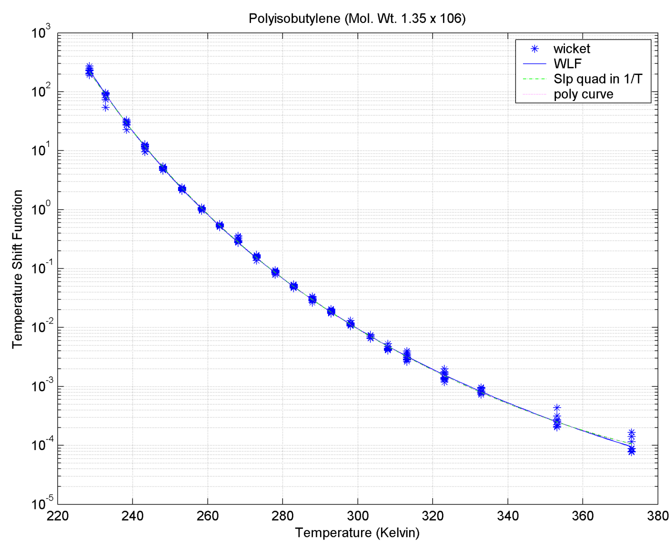

Figure 13: The Temperature Shift Function for Polyisobutylene

The set of complex modulus data itself implicitly defines the TSF, and one purpose of any method to smooth, interpolate and model a set of complex modulus data is to facilitate this. The present method is well founded on mathematical rigor and is believed to be insensitive to limited frequency and temperature ranges, data scatter, etc.

It remains to smooth, interpolate and model the temperature shift as a function of temperature. This is done by a best fit of equations to the TSF points. Figures 11-13 present the TSF points as a function of temperature as well as three equations (the WLF, the Slope as a Quadratic in (1/T), and a fourth order polynomial) which have been fitted to the data. Figure 14 is the plot of the temperature shift function (TSF) plotted vs 1000/T for the VEM processed in the present effort; because this does not appear to be a straight line, the Arrhenius equation is not considered further in the present effort. The usual International Plot Nomograms[12] with solid lines/curves indicating the experimental range are presented as Figure 16. Only the Nomogram is of direct interest to designers, while the TSF, the slope, the

AAE, and other quantities are of more detailed or specialized interest. The slope of the TSF is presented in Figure 15 and compared with those from a previous investigation[13].

The form of the Ratio Model makes interconversion to other dynamic mechanical properties such as molecular weight distribution, relaxation modulus, creep compliance, and relaxation and retardation spectra convenient[1].

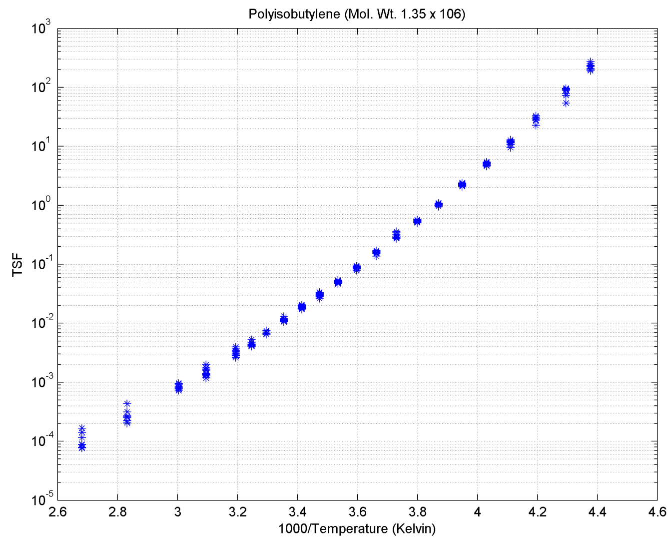

Figure 14: The TSF vs 1/T for VEM Polyisobutylene

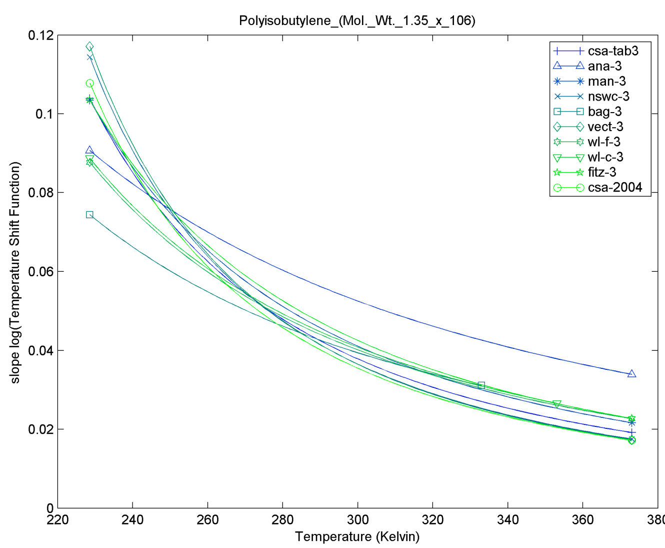

Figure 15: The Slope of the Temperature Shift Function for Polyisobutylene

DISCUSSION

Typically, when a set of complex modulus data is developed, there will be scatter in the measurements. Therefore, smoothing is essential. The set of data does not define a continuous function; therefore, interpolation is required. Smoothing and interpolation start with the Analytic Wicket, presently a series of splines, representing the data region and reasonable extrapolations into the skirts. The extrapolations are necessary because the equation modeling the complex modulus as a function of reduced radian frequency cannot be truncated at the end of the data region. It is assumed that the Analytic Wicket is sufficiently accurate in fully characterizing the set of data. In the data region, a series of splines is fitted to the center and slope of the band of data, thereby both smoothing and interpolating the experimental region. The fitting and extrapolations are automated and goodness of fit is somewhat subjective, especially at the ends of the data region. In general, the center half or three-fourths or so of a range of data is relatively easy to fit to some equation whereas the ends can be quite difficult and somewhat arbitrary. The scatter in the points in the wicket plot will show up again in both the TSF plot and the nomogram (see Figures 5, 13 & 16). Any future efforts for improvement should be initially directed at the Analytic Wicket.

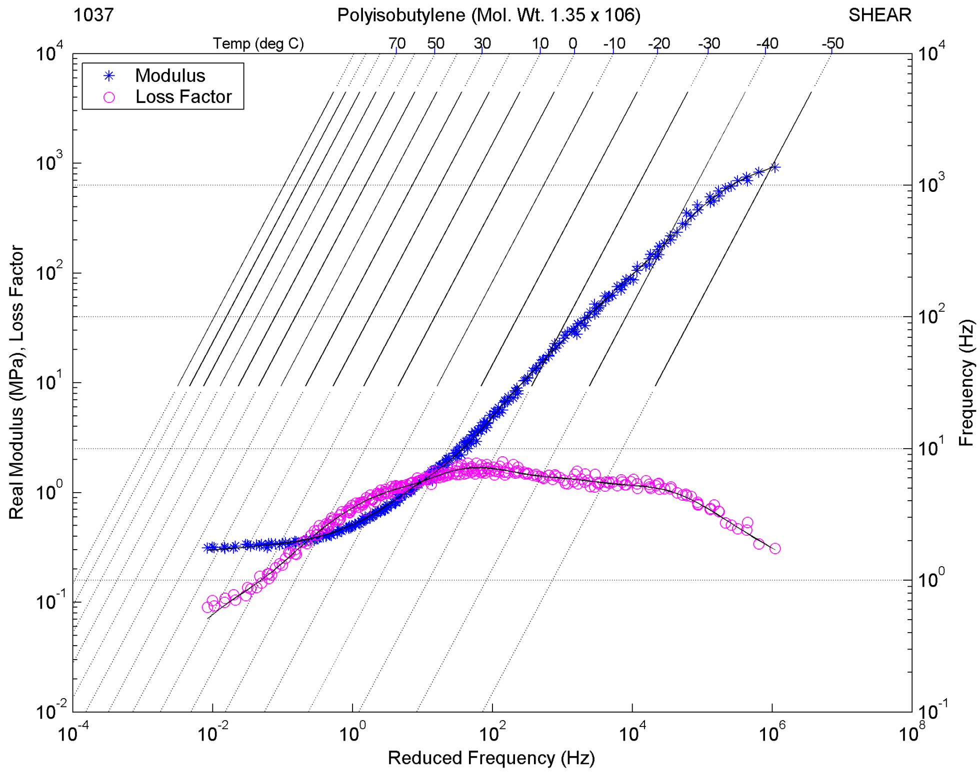

Figure 16: The Nomogram for Polyisobutylene

Once the wicket plot points are edited and the Analytic Wicket accepted, the process is fully automated. The form of the Ratio Model facilitates mapping, which consists of initiation and iteration phases. After convergence, the computer calculates the TSF points as a function of temperature and generates a polynomial TSF curve, which smoothes and interpolates the TSF as a function of temperature. The TSF points and equations are shown in Figure 13 together with equations which smooth and interpolate. There is scatter in the middle of the data region as well as at the ends. The slope of the present TSF is presented in Figure 15 together with those from a previous study. Examination of the TSF reveals that there is some subjectiveness and arbitrariness at the very ends in the TSF fit and therefore also in the slope. None of the other slopes in Figure 15 agree closely with the present one over the full range of temperature. The apparent activation energy (AAE) is of interest to some investigators and could be calculated easily but is not presented in the present document. The present approach fits polynomials to the TSF and plots TSF, slope, and AAE; the order is increased until there is too much waviness in one or more of the plots. A sixth order polynomial seems most appropriate based on processing approximately 10 sets of data. There is no apparent advantage to using historical TSF equations. The form of the Ratio Model makes interconversion to other dynamic mechanical properties such as molecular weight distribution, relaxation modulus, creep compliance, and relaxation and retardation spectra convenient [1]. At this juncture, all plots have been generated and are available for display at the option of the operator. The nomogram smoothes and interpolates with respect to frequency. The purpose for which the set of data is intended will dictate whether or not the smoothing, interpolation, and modeling is sufficiently accurate. For purposes of damping design, the center of the transition is of most concern.

SUMMARY

This new approach of smoothing, interpolating, and modeling (SIM) a set of complex modulus data and its temperature shift function (TSF) is a network of mutually complementary elements. One key of the system is the wicket plot. Initially, it is used to display the set of data under consideration. It can be used to edit individual points and reveal conspicuously bad data; but a tight wicket plot does not guarantee that the data is accurate. In this new approach, the wicket plot plays a further role which is rooted in the mathematics of linear systems. The Analytic Wicket may be considered to be one function, ie, material loss factor as a function of modulus magnitude; it may also be considered to be two functions, namely material loss factor and modulus magnitude, of the parameter, arc length, s. From systems theory, it is known that these two functions are also two components of a complex valued function of one independent variable, reduced radian frequency. Reduced radian frequency in turn is a function of two independent variables, radian frequency and temperature, and is a product of radian frequency and the temperature shift function.

Another key is the form of the model or complex valued function (i.e., the complex modulus), namely the Ratio Model, which is a ratio of polynomials of first order factors with the numerator and the denominator being the same order. One pair of first order factors, one in the numerator and the other in the denominator, form one "step" with respect to Bode Diagram considerations. The Ratio Model possesses three major benefits: 1) it intrinsically guarantees that the interrelationships of linear systems are satisfied, 2) it facilitates the mapping, and 3) it facilitates the interconversion to other dynamic mechanical properties. The mapping consists of an initialization phase and an iteration phase and is used to determine values for the parameters in the Ratio Model. The basic fractional derivative equation for complex modulus is critical to the initialization process. One characteristic of complex modulus is that the loss factor is strongly dependent on the slope of the modulus magnitude as a function of reduced radian frequency. The iteration process is based on this characteristic. The Ratio Model is used to calculate modulus magnitude and loss factor at each “step;” and the Analytic Wicket is used to calculate the loss factor corresponding to the modulus from the Ratio. If the two values for loss factor are not identical, the slope of the Ratio modulus is changed appropriately.

Still another key is the use of the perpendicular distance from each experimental data point to the wicket plot and the associated value of reduced radian frequency to calculate the value of the temperature shift function for that data point. Another key is the use of modern computational power which enables utilization of models having a large number of parameters.

The present approach is interactive and highly automated. It facilitates communication, is useful to the designer, is fair to the material supplier and tester, and puts pressure on the damping industry to make further improvements and advancements within the limits of economic practicality.

Computerized modeling greatly facilitates storage, retrieval, and dissemination of the dynamic mechanical properties of a damping polymer. These are crucial factors in the further advancement and application of damping technology. The present method is well founded on mathematical rigor and is believed to be insensitive to limited frequency and temperature ranges, data scatter, etc.

It appears that a quantum leap of maturity, accuracy, and efficiency has been achieved.

ACKNOWLEDGEMENT

The development reported herein occurred during several programs over several years under sponsorship of the U.S. Air Force, which is gratefully acknowledged.

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